Swapping entangled Kondo resonances in parallel-coupled double quantum dots

Guang-Ming Zhang[1,2], Rong Lü[1], Zhi-Rong Liu[2], and Lu Yu[3]
[1] *Center for Advanced Study, Tsinghua University, Beijing 100084, China;*
[2] *Department of Physics, Tsinghua University, Beijing 100084, China;*
[3] *Interdisciplinary Center of Theoretical Studies and Institute of Theoretical Physics, CAS, Beijing 100080, China.*
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Strong electron and spin correlations are studied in parallel-coupled double quantum dots with interdot spin superexchange J. In the Kondo regime with *degenerate* dot energy levels, a coherent transport occurs at zero temperature, where two entangled (bonding and antibonding) resonances are formed near the Fermi energy. When increasing J or the dot-lead parallel-coupling *asymmetry* ratio Γ_2/Γ_1, a swap between two entangled resonances occurs and the line shapes of the linear conductance are interchanged. The zero-bias differential conductance shows a peak at the critical values. Such a peculiar effect with the virtue of many-body coherence may be useful in future quantum computing.

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A large number of proposals have been made to materialize quantum bits (qubits) and quantum computing. Among these proposals, coupled quantum dot (QD) systems are particularly attractive.[1] The spin degree of freedom of the localized electrons on the dots is considered as a qubit due to the comparatively long coherence time. A key challenge is the construction of coupled double QD (DQD) to perform a swap operation, *i.e.* exchanging the electron spin states on the two dots. When the square root of a swap operation is combined with other isolated qubit rotations, a quantum controlled-NOT gate can be built and any quantum algorithms can be implemented.[2] In the coupled DQD, two local electrons form a singlet state. It has been proposed that the swap operation can be realized by tuning the time-dependent interdot spin superexchange (ISS) $J(t)$ from positive to negative, flopping the singlet and triplet states.[1, 3]

In this Letter, we propose a simple and reliable mechanism to perform such a swap process in a parallel-coupled DQD at low temperatures. It has been well-established that under the Coulomb blockade with odd number electrons on a single QD, a quantum coherent many-body (Kondo) resonance is formed near the Fermi energy in the dot density of states (DOS) [4]. The Kondo effect for even number electrons on a single multilevel dot and possible phase transitions between singlet and triplet states have been considered for both "vertical"[5] and "lateral" [6, 7, 8, 9] configurations. For the coupled DQD with degenerate energy levels, the Kondo behavior and the ISS interplay and strongly compete, as seen in the bulk two-impurity Kondo problem,[10] and a question arises whether there exists a spin entangled state composed of the coherent Kondo resonances.[11] Previous experimental and theoretical studies have mainly focused on the serial-coupled DQD [12, 13, 14, 15, 16, 17, 18, 19], except for Ref. 9, 19. However, it has been recently realized that the serial geometry is *unsuitable* for studying this competition experimentally and a direct evidence for observing spin entanglement between the dot local electrons could be sought in the parallel coupled configuration.[20] It has thus motivated us to investigate whether and how this competition manifests itself in the coherent transport through DQD in the parallel configuration.

For a degenerate DQD with ISS, a special dot-lead coupling configuration (see Fig. 1) is considered. By increasing the dot-lead coupling asymmetry ratio Γ_2/Γ_1 ($\Gamma_{1,2} = \pi\rho_f V_{1,2}^2$), where ρ_f is the DOS at the Fermi level and $V_{1,2}$ is the dot-lead hopping integrals, the dot local electrons couple to the right and left electrodes can be transformed from serial ($\Gamma_2 = 0$) to symmetric parallel-coupled configuration ($\Gamma_2 = \Gamma_1$). We generalize the slave-boson mean field (MF) theory [21] to take into account both electron and spin correlations *simultaneously*. Using an entanglement order parameter (EOP) Δ_f and the asymmetry ratio Γ_2/Γ_1 to describe the entanglement between the local electron spins, we find that two entangled bonding and antibonding Kondo resonances are formed very close to the Fermi energy. When increasing the ISS or the dot-lead coupling asymmetry ratio, the EOP can change sign at a critical value. As a result, the bonding and antibonding resonances swap, or equivalently, the singlet and triplet levels interchange and the zero-bias differential conductance displays a peak at the critical value. Importantly such a swap effect occurs *only* when the dot-lead parallel couplings are *asymmetric*, *i.e.* $0 < \Gamma_2/\Gamma_1 < 1$ and the gate voltage controlling the interdot electron hopping is fine tuned.

We describe the coupled DQD system as two Anderson magnetic impurities with *degenerate* levels and infinite on-site Coulomb repulsion, and an antiferromagnetic(AF) spin superexchange between two local electron spins is generated by the second order perturbation in the interdot electron tunneling. The model Hamiltonian is given by

$$H = \sum_{\mathbf{k},\sigma;\alpha=L,R} \epsilon_{\mathbf{k},\alpha} C^{\dagger}_{\mathbf{k},\sigma,\alpha} C_{\mathbf{k},\sigma,\alpha} + \sum_{\sigma;i=1,2} \epsilon_d f^{\dagger}_{i,\sigma} f_{i,\sigma}$$
$$+ \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\sigma} \Big[\Big(V_1 f^{\dagger}_{1,\sigma} b_1 + V_2 f^{\dagger}_{2,\sigma} b_2 \Big) C_{\mathbf{k},\sigma,L}$$

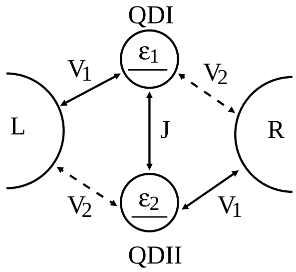

FIG. 1: Configuration of the coupled double quantum dots with asymmetric couplings to the left and right electrodes. Two degenerate dot levels ($\epsilon_1 = \epsilon_2$) are coupled by an AF spin superexchange with strong on-site Coulomb repulsion.

$$+\left(V_2 f_{1,\sigma}^\dagger b_1 + V_1 f_{2,\sigma}^\dagger b_2\right) C_{\mathbf{k},\sigma,R} + h.c.\Big]$$
$$+J\left(2\mathbf{S}_1\cdot\mathbf{S}_2 + \frac{1}{2}\right), \tag{1}$$

where N is the total number of electrons, the slave-boson representations $d_{i,\sigma} = b_i^\dagger f_{i,\sigma}$ have been used to describe the local electrons on each QD (b_i and $f_{i,\sigma}$ denote the respective hole and electron occupied states), and the local constraints $b_i^\dagger b_i + \sum_\sigma f_{i,\sigma}^\dagger f_{i,\sigma} = 1$ have to be imposed [21]. $\mathbf{S}_1$ and $\mathbf{S}_2$ correspond to the spin density operators of the dot local electrons, characterized by $S_i^\alpha = \sum_{\sigma,\sigma'} f_{i,\sigma}^\dagger \tau_{\sigma,\sigma'}^\alpha f_{i,\sigma'}$ with τ^α ($\alpha = x, y, z$) the Pauli matrices. Here, we are only concerned with the equilibrium ($\epsilon_{\mathbf{k},L} = \epsilon_{\mathbf{k},R}$) properties. A similar coupling configuration of the DQD model has been studied in the noninteracting case.[22] Since the ISS interaction can be written in an SU(2) singlet form [23]

$$J\sum_{\sigma,\sigma'} f_{1,\sigma}^\dagger f_{1,\sigma'} f_{2,\sigma'}^\dagger f_{2,\sigma} = -J\sum_{\sigma,\sigma'} : f_{1,\sigma}^\dagger f_{2,\sigma} f_{2,\sigma'}^\dagger f_{1,\sigma'} :$$

in the MF approximation, an EOP $\Delta_f = \sum_\sigma \langle f_{1,\sigma}^\dagger f_{2,\sigma}\rangle$ can be introduced to describe the spin singlet between the local electrons on two separate dots. As in the usual treatment of the Anderson impurity model at $T = 0$, the bosonic operators are replaced by their expectation values and the local constraints by the Lagrangian multipliers λ_i. It has been established that the slave-boson MF treatment captures the basic Kondo physics for the single-impurity Anderson model at low temperatures, and such a theory becomes exact for large local spin degeneracy.[21] In the presence of degenerate dot energy levels, we expect to have $\lambda_1 = \lambda_2 = \lambda$ and $b_1 = b_2 = b_0$, namely, the degeneracy of the dot energy levels can *only* be lifted by the ISS interaction. Thus, an effective model Hamiltonian is obtained

$$\begin{aligned} H_e &= \sum_{\mathbf{k},\sigma;\alpha} \epsilon_{\mathbf{k}} C_{\mathbf{k},\sigma,\alpha}^\dagger C_{\mathbf{k},\sigma,\alpha} + (\widetilde{\epsilon}_d - J\Delta_f)\sum_\sigma \alpha_\sigma^\dagger \alpha_\sigma \\ &\quad +(\widetilde{\epsilon}_d + J\Delta_f)\sum_\sigma \beta_\sigma^\dagger\beta_\sigma + 2\lambda\left(b_0^2 - 1\right) + J\Delta_f^2 \\ &\quad +\frac{(\widetilde{V}_1+\widetilde{V}_2)}{\sqrt{2N}}\sum_{\mathbf{k},\sigma}\left[\alpha_\sigma^\dagger\left(C_{\mathbf{k},\sigma,L} + C_{\mathbf{k},\sigma,R}\right) + h.c.\right] \\ &\quad +\frac{(\widetilde{V}_1-\widetilde{V}_2)}{\sqrt{2N}}\sum_{\mathbf{k},\sigma}\left[\beta_\sigma^\dagger\left(C_{\mathbf{k},\sigma,L} - C_{\mathbf{k},\sigma,R}\right) + h.c.\right], \end{aligned}$$

where $\widetilde{\epsilon}_d = \epsilon_d + \lambda$ and $\widetilde{V}_i = b_0 V_i$ are two renormalized parameters, and two canonical modes of bonding and antibonding have been introduced by $\alpha_\sigma = \frac{1}{\sqrt{2}}\left(f_{\mathbf{1},\sigma} + f_{\mathbf{2},\sigma}\right)$ and $\beta_\sigma = \frac{1}{\sqrt{2}}\left(f_{\mathbf{1},\sigma} - f_{\mathbf{2},\sigma}\right)$. The difference between the bonding and antibonding energies are just given by $2J\Delta_f \equiv J_{eff}$. Actually, J_{eff} also corresponds to the effective energy splitting of the spin singlet and triplet states formed by the renormalized local electrons on the dots. Thus, a singlet-triplet transition can occur when the EOP Δ_f changes sign, instead of reversing the sign of J.

When a Nambu spinor $\Phi_\sigma^\dagger = \left(f_{1,\sigma}^\dagger, f_{2,\sigma}^\dagger\right)$ is defined, the Fourier transform of the retarded Green's function $-\langle T_\tau \Phi_\sigma(\tau)\Phi_\sigma^\dagger(\tau')\rangle$ can be derived as

$$\mathbf{G}_f(\omega) = \frac{\left[\omega - \widetilde{\epsilon}_d + i(\widetilde{\Gamma}_1 + \widetilde{\Gamma}_2)\right] - \left[J\Delta_f + 2i\sqrt{\widetilde{\Gamma}_1\widetilde{\Gamma}_2}\right]\sigma_x}{\left[\omega - \widetilde{\epsilon}_\alpha + i\widetilde{\Gamma}_\alpha\right]\left[\omega - \widetilde{\epsilon}_\beta + i\widetilde{\Gamma}_\beta\right]},$$

where σ_x is the Pauli matrix, and the DOS on each QD is given by $A_f(\omega) = \frac{1}{2\pi}\left[\frac{\widetilde{\Gamma}_\alpha}{(\omega-\widetilde{\epsilon}_\alpha)^2+\widetilde{\Gamma}_\alpha^2} + \frac{\widetilde{\Gamma}_\beta}{(\omega-\widetilde{\epsilon}_\beta)^2+\widetilde{\Gamma}_\beta^2}\right]$, corresponding to a superposition of the bonding and antibonding resonances lying at energies $\widetilde{\epsilon}_{\alpha,\beta} = (\widetilde{\epsilon}_d \mp J\Delta_f)$ with renormalized hybridization widths $\widetilde{\Gamma}_{\alpha,\beta} = b_0^2\pi\rho_f\left(V_1 \pm V_2\right)^2$. Actually, these are two entangled resonances with many-particle coherence, and we will refer to them as entangled bonding and antibonding Kondo resonances. At the symmetric parallel-coupling $\Gamma_2 = \Gamma_1$, only the bonding combination of the conduction electrons, i.e. $(C_{\mathbf{k},\sigma,L} + C_{\mathbf{k},\sigma,R})$ couples to the localized electrons, and the antibonding combination $(C_{\mathbf{k},\sigma,L} - C_{\mathbf{k},\sigma,R})$ are completely dropped out. [9]

To determine the MF order parameters b_0^2 and Δ_f, the corresponding self-consistent equations $\sum_\sigma\langle f_{i,\sigma}^\dagger f_{i,\sigma}\rangle = 1 - b_0^2$ and $\sum_\sigma\langle f_{1,\sigma}^\dagger f_{2,\sigma}\rangle = \Delta_f$, are rewritten as

$$1 - b_0^2 = \frac{1}{\pi}\left[\tan^{-1}\left(\frac{\widetilde{\Gamma}_\alpha}{\widetilde{\epsilon}_\alpha}\right) + \tan^{-1}\left(\frac{\widetilde{\Gamma}_\beta}{\widetilde{\epsilon}_\beta}\right)\right], \tag{2}$$
$$\Delta_f = \frac{1}{\pi}\left[\tan^{-1}\left(\frac{\widetilde{\Gamma}_\alpha}{\widetilde{\epsilon}_\alpha}\right) - \tan^{-1}\left(\frac{\widetilde{\Gamma}_\beta}{\widetilde{\epsilon}_\beta}\right)\right], \tag{3}$$

where the first equation represents the total quasiparticle occupations on bonding and antibonding energy levels, while Δ_f corresponds to the difference between these two occupations as follows from the Friedel sum

rule. Moreover, a third self-consistent equation from $\langle \partial_\tau b_i \rangle = \langle [b_i, H] \rangle = 0$ is needed, yielding

$$\widetilde{\epsilon}_d - \epsilon_d = \frac{1}{\pi b_0^2}\left[\widetilde{\Gamma}_\alpha \ln\frac{D}{T_\alpha} + \widetilde{\Gamma}_\beta \ln\frac{D}{T_\beta}\right], \qquad (4)$$

where two characteristic energy scales are formally defined as $T_{\alpha(\beta)} = \sqrt{(\widetilde{\epsilon}_d \mp J\Delta_f)^2 + (b_0^2 \pi \rho_f)^2 (V_1 \pm V_2)^4}$ with D as the bandwidth of the conduction electrons in leads. We have to stress that these two energy scales can not be directly related to the Kondo temperatures defined in the multilevel QD system.[6, 9] To find the saddle point solution numerically, we choose $\Gamma_1 = 1$ as the energy unit and $D = 100$.

In the Coulomb blockade regime for each dot, the degenerate dot energy level is set by $\epsilon_d = -6$, far below the Fermi energy. We find that T_α grows as increasing Γ_2, while T_β is a small constant ($T_\beta < T_\alpha$). For a given value of Γ_2, both T_α and T_β are almost independent of J. In the parallel-coupled DQD with a tunable ISS, the electron occupation on each dot *strongly* depends on parameters Γ_2 and J. Given a dot-lead coupling asymmetry ratio Γ_2, we find that the MF value of Δ_f grows as J increasing and changes sign at a critical value J_c. When Δ_f reverses sign, the relative position of the bonding and antibonding energies of the renormalized dot energy levels are switched, *i.e.*, the quantum spin states on QDs are swapped. Similarly, for a fixed value of J, there also exists a critical value of the dot-lead coupling asymmetry ratio ($0 < \Gamma_{2,c} < 1$), where Δ_f changes sign. Such a sign change effect signals the existence of two different regimes in the *asymmetric* parallel-coupled DQD system. In Fig.2, we display EOP Δ_f as functions of the ISS J and the ratio of the dot-lead couplings Γ_2. Actually, the dramatic effect of Δ_f is not sensitive to the parameter ϵ_d as long as the condition $|\epsilon_d| > \Gamma_2$ is satisfied. In Fig.2c, a phase diagram is given in the three-parameter space $(\epsilon_d, \Gamma_2, J)$. Moreover, we evaluated the dot electron DOS for $\epsilon_d = -6$ and $\Gamma_2 = 0.6$ with different ISS, shown in the left column of Fig.3. When $J = 0.1$, Δ_f has a very small value, and the entangled bonding and antibonding resonances are very close to each other and hardly distinguishable in Fig.3a. For $J = 0.205$, Δ_f reaches its largest value and the entangled bonding resonance appears below the Fermi energy (Fig.3b). When $J = 0.210$, Δ_f changes sign and the bonding resonance state swaps its position from below to above the Fermi level. At $J = 0.3$, the bonding and antibonding resonances emerge again. In this process, a sharp and narrow entangled resonance always stands close to the Fermi level.

From the Landauer formula, the linear conductance can also be calculated

$$G(\omega) = \frac{2e^2}{h}\mathrm{Tr}\left[\mathbf{G}_f(\omega - i0^+)\mathbf{\Gamma}_R \mathbf{G}_f(\omega + i0^+)\mathbf{\Gamma}_L\right], \quad (5)$$

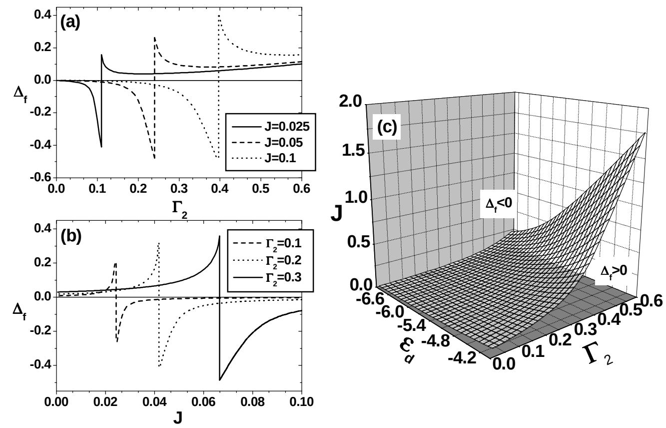

FIG. 2: The order parameter Δ_f in the Kondo regime ($\epsilon_d = -6$) as functions of the asymmetry ratio of the dot-lead couplings Γ_2 in (a) and the ISS J in (b). The ground state phase diagram is given in (c). $\Gamma_1 = 1$ is as the energy unit.

where $\mathbf{G}_f(\omega + i0^+)$ and $\mathbf{G}_f(\omega - i0^+)$ represent the retarded and advanced Green's functions, and $\mathbf{\Gamma}_R = 2b_0^2\begin{pmatrix} \Gamma_2, & \sqrt{\Gamma_1\Gamma_2} \\ \sqrt{\Gamma_1\Gamma_2}, & \Gamma_1 \end{pmatrix}$ and $\mathbf{\Gamma}_L = 2b_0^2\begin{pmatrix} \Gamma_1, & \sqrt{\Gamma_1\Gamma_2} \\ \sqrt{\Gamma_1\Gamma_2}, & \Gamma_2 \end{pmatrix}$ are two matrices related to the asymmetric dot-lead couplings. The corresponding results are delineated in the right column of Fig.3. For the intermediate couplings of J, the linear conductance displays a Lorentzian conductance peak centered at the bonding energy and a Fano resonance at the antibonding energy (Fig.3b'). The latter arises due to the presence of bound states of DQD embedded in the conduction band continuum. However, when the EOP Δ_f changes sign, these two characteristic line shapes are switched (seen in Fig.3c'). For a smaller value of J in Fig.3a', the Fano resonance with a small transmission is an anti-resonance at the Fermi energy, because of the destructive quantum interference between different pathways through QDs. As J is large in Fig.3d', there is a progressive increase of the width of the bonding resonance. For the serial-coupled ($\Gamma_2 = 0$) and symmetric parallel-coupled ($\Gamma_2 = \Gamma_1$) DQD, these swapping features do not appear. To make contacts with experiments directly, we extract the zero-bias differential conductance $G(\omega = 0)$ as functions of the asymmetric coupling parameters Γ_2 and ISS J for a given value of $\epsilon_d = -6$, displayed in Fig.4a and 4b. Surprisingly, we find that the differential conductances have maxima *precisely* at the critical couplings for swap. The appearance of such sharp conductance peaks can be explained by the majority occupation of the bonding quasiparticle states across the Fermi level during the swap process. We should point out that the singlet-triplet transition discussed here is very different from

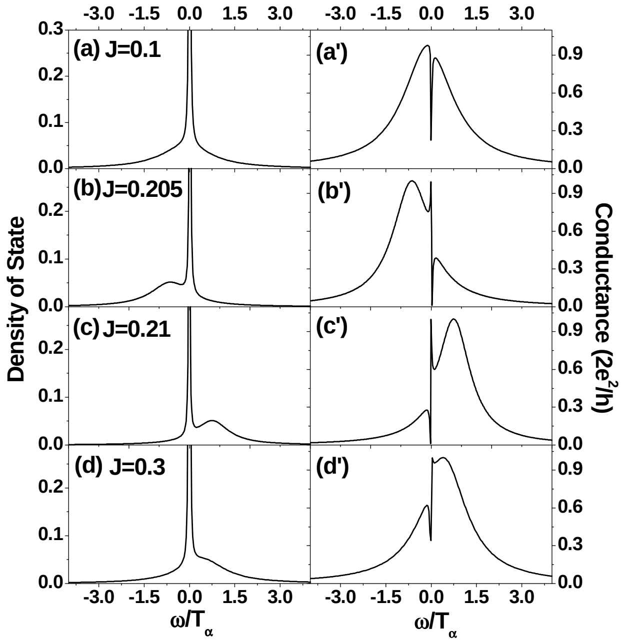

FIG. 3: The dot DOS and the corresponding linear conductance for different interdot AF spin superexchange J with a given asymmetry ratio of the dot-lead couplings $\Gamma_2 = 0.6$ and degenerate dot energy levels $\epsilon_d = -6$.

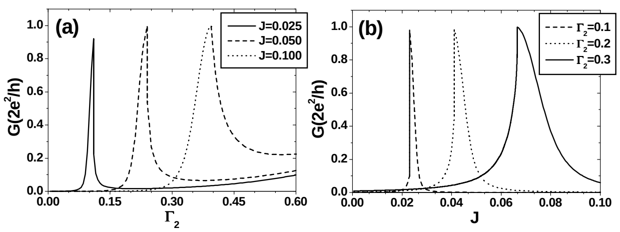

FIG. 4: The zero-bias differential conductance as functions of the asymmetry ratio of coupling parameters Γ_2 and the ISS J with degenerate dot energy level $\epsilon_d = -6$.

what was considered in multilevel dots [6, 7, 8, 9], where the coupling parameter symmetry excludes completely the antibonding channel of the conduction electrons, so the swap effect does not appear there. It is true that the quantum fluctuations beyond the MF description may change detailed behavior near the swap point, but the existence of the swap itself is a robust effect, because two MF solutions with opposite sign of Δ_f are stable.

To conclude, in a degenerate parallel-coupled DQD with asymmetric parallel couplings, two entangled bonding and antibonding resonances are formed close to the Fermi energy in the Kondo regime of each dot. A swap effect between two resonances has been found, leading to a sharp peak centered at the critical coupling in the zero-bias differential conductance. To observe such a peculiar effect in experiments, one has to fine tune the corresponding gate voltage controlling the interdot electron hopping or the dot-lead coupling asymmetry ratio in a parallel-coupled DQD system. Moreover, this effect will lead to a practical and reliable mechanism to construct the quantum gate for the future quantum computing.

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